Influence of copper single crystal structures on the reflection of low energy hydrogen and helium ions

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INTRODUCTION AND SUMMARY.

In recent years the reflection of low energy (≲10 keV) noble gas ions has been applied as an investigation method to study different characteristic features of the outermost layer of single crystal surfaces (1). By carefully studying the energy spectra of singly and multiply reflected noble gas ions, information can be obtained about for instance:

- the elemental compositions of the outermost surface layer (2,3,4,5)
- the position of adsorbed atoms, relative to the target atoms (5,6)
- structural features on the surface (7,8)
- thermal vibrations of surface atoms (9,10)

All these investigations, concerned with the top layer of a surface, can be made because of the high neutralization probability of low energy noble gas ions at solid surfaces. As a result reflected *ions* mainly originate from the outermost layer. Ions reflected from deeper layers in the crystal are considered to emerge from the surface as neutrals and thus escape the usually applied ion detection methods. Apparently therefore, the reflection of low energy noble gas ions, being the main subject of investigations of our research group (11,12,13, 14), provides unique information about the outermost layer of a solid surface. However, information about the different processes going on just below the surface during the ion bombardment as for instance noble gas ion entrapment (15,16) usually will escape detection.

In order to study such sub-surface processes going along with the bombardment of low energy noble gas ions, having range profiles extending up to some tens of Angströms below the surface at most (17), one really needs a method which can give more specific information about the *first few* layers. A method which has been applied successfully in high energy implantation and damage studies, is the combination channeling - backscattering of MeV light (H^+, He^+) ions (18). However, when information about only the first few layers is required, this MeV-method fails because of a lack of sufficient depth resolution. For high primary H^+ or He^+ energies namely the obtained information always is an average over about some tens of Angströms or more (19). At lower primary energies, however, because of a relative increase of the electronic stopping power, this depth resolution in principle can be improved to even some Angströms by using high resolution electrostatic analysers. It follows that for the study of the first few layers of a crystal surface, using the combination channeling - backscattering, primary ion energies of just some keV would be sufficient when only the range of these ions (10-100 Å/keV) had to be taken into account. However, in order to define a depth resolution in such experiments, one must be able to relate the energy of the backscattered ions unambigiously to the depth below the surface from which scattering takes place. This in turn is only possible when the so-called "single reflection approximation" holds, i.e. when the chance of reflection back into the vacuum through a multiple collision process can be neglected with respect to the chance of reflection via one single collision with a target atom. In view of scattering cross section considerations this implies, that light primary particles with energies of at least 10 keV should be applied.

Summarizing the above discussion one may state that the combination channeling - backscattering of ∿ 10 keV light ions in principle should be an attractive analysing method in those investigations where interest is focused on the first few layers of single crystal surfaces. So far, however, little data on the channeling and reflection of low energy light ions from single crystals have been presented in literature (20). In view of this circumstance it will be obvious that investigations on the analysing capabilities of the just mentioned method have to be preceded by a study of the basic aspects in this field of interest. Hence, the research which resulted in the underlying thesis, began with a preliminary study of the channeling and reflection characteristics of low energy ($\lesssim$10 keV) light ions (H^+, He^+) in a copper (001) single crystal (21). From these measurements it appeared, that the present apparatus, primarily designed for the study of the (multiple) relection of noble gas ions from single crystal surfaces (22), was not well suited to study channeling effects under optimum conditions. Therefore we started the design and construction of a very sophisticated channeling-compatible apparatus, which at this moment is in its final test stage (23).

With the present apparatus, however, it was still possible to study a number of interesting aspects of low energy light ion reflection. Thus, it appeared that under certain circumstances the reflection of H^+ and He^+ ions was seriously influenced by the focusing action of the so-called surface "semi-channels", formed by the atomic rows of the first and second crystal layers. This fascinating effect, called by us "wedge-focusing", has been extensively investigated (24,25,26) and actually has become the main subject of this thesis.

A theoretical basis for the "wedge-focusing" phenomenon has been outlined in chapter I. On the basis of computer simulations, the so-called "shadow-model" for ion scattering has been applied. This model gives a qualitative description of different aspects of low energy light ion scattering, as for instance: the chain effect, the channeling and the wedge-focusing effect.

With regard to the chain effect, characteristic differences show up when different interatomic potentials are applied.

In the section on channeling it is shown that different parts of the ion beam, when incident along a low index direction, have to be considered separately, because they are scattered in different ways. Furthermore it appears that dechanneling always occurs when adequate interaction models are applied.

Finally it turns out that under wedge-focusing conditions the reflected yield from the second layer strongly increases with respect to reflection from other crystal layers.

In low energy proton scattering experiments, because of yield considerations, it is often attractive to use the H_2^+ or H_3^+ ion species instead of H^+. In chapter II, investigations have been made to check up to what extend proton reflection indeed can be simulated by using H_2^+ or H_3^+ as incident ions and analysing the reflected protons. Differences in the reflection behaviour of protons resulting from the interaction of H^+, H_2^+ and H_3^+ ions with the copper target have been studied on the basis of the position and width (FWHM) of the "surface" peak in the energy spectrum of the reflected protons. It appears that for incident H^+, H_2^+ and H_3^+ ions having the same energy per nucleon, the proton surface peak in the reflected energy spectrum occurs at approximately the same energy value. The FWHM of this peak however strongly differs for the different primary species.

In chapter III the results are presented of an experimental study of the influence of surface semi-channels on the reflection of low energy ($\lesssim$10 keV) H^+, H_2^+ and He^+ ions from copper single crystals with the attention focused on the wedge-focusing effect.

Measurements are performed on two different semi-channel types namely the <110> structures on both a Cu

(001) and Cu (111) crystal surface.

As a result of the wedge-focusing effect, in the energy spectrum of reflected He^+ ions, reflection from the first and the second crystal layer do show up as separate peaks, which in turn opens the possibility to obtain information on the electronic energy loss as experienced by incident ions on their way through the semi-channel.

In addition it appears to be possible to obtain supplementary information on the reflection characteristics of H^+ from the first and second layer by comparison with similar He^+ measurements.

Differences between experimentally determined crystal orientations for wedge-focusing and those obtained from the theoretical model as described in chapter I will be discussed in terms of potential choice and surface relaxation.

In chapter IV the experimental results are presented of some preliminary investigations on the influence of axial and planar channeling and blocking effects (including double-alignment) on the reflection behaviour of low energy ($\leq$10 keV) protons, resulting from H^+ and H_2^+ ion beams incident on the (001) surface of a copper single crystal.

From these measurements it seems to be justified to conclude that, for primary energies $\sim$10 keV, the combination channeling-backscattering of protons might be quite well applicable for foreign atom location studies in the top few layers of single crystal surfaces.